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13. ABSTRACT (Maximum 200 words)

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Report Title

Enhanced Interface Mechanics for Multimaterial FEM

ABSTRACT

Multi-material Eulerian and arbitrary Lagrangian-Eulerian methods were originally developed for solving hypervelocity impact problems, but they are attractive for solving a broad range of problems having large deformations, the evolution of new free surfaces, and chemical reactions. The contact, separation, and slip between two surfaces have traditionally been addressed by the mixture theory, however the accuracy of this approach is severely limited. To improve the accuracy, an extended finite element formulation is developed and example calculations are presented. As a side benefit, the mixture theory is eliminated from the multi-material formulation, eliminating the issues associated with the equilibration time between adjacent materials. By design, the new formulation is relatively simple to implement in existing multi-material codes, parallelizes without difficulty, and has a low memory burden.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Vitali, E. and D. J. Benson, "An extended finite element formulation for contact in multi-material arbitrary Lagrangian-Eulerian calculations," International Journal for Numerical Methods in Engineering, V67, 1420-1444, (2006).

Number of Papers published in peer-reviewed journals: 1.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

(c) Presentations

"An extended finite element method for contact in Eulerian finite element analysis." 7th World Congress on Computational Mechanics, Los Angeles, CA, July 16-22, 2006

"Contact formulations for Eulerian finite element methods." SIAM Conference on Financial Mathematics and Engineering, Boston, MA, July 9-12, 2006

"An extended finite element method for contact in multi-material Eulerian hydrocodes." 17th US Army Symposium on Solid Mechanics, April 2-5, 2007

"Contact methods for multi-material Eulerian and ALE finite element analysis" Plenary lecture, 12th Annual Conference on Computational Engineering and Science, Tokyo, Japan, May 25-27, 2007

Number of Presentations: 4.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

(d) Manuscripts

Number of Manuscripts: 0.00

Number of Inventions:

Graduate Students

NAME	PERCENT_SUPPORTED
Efrem Vitali	0.49
FTE Equivalent:	**0.49**
Total Number:	**1**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
David Benson	0.05	No
FTE Equivalent:	**0.05**	
Total Number:	**1**	

Names of Under Graduate students supported

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This section only applies to graduating undergraduates supported by this agreement in this reporting period

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Names of Personnel receiving masters degrees

NAME	
Efrem Vitali	
Total Number:	**1**

Names of personnel receiving PHDs

NAME	
Efrem Vitali (Spring Quarter, 2007)	
Total Number:	**1**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

An Extended Finite Element Method for Contact in Multi-Material Eulerian Hydrocodes

David J. Benson & Efrem Vitali

Dept. of Mechanical and Aerospace Engineering

University of California, San Diego

La Jolla, CA

Research supported by Army Research Organization Grant

DAAD19-02-1-0266

Objective

- Eliminate the last major limitation of multi-material Eulerian FEM and FD formulations by the development of a general contact methodology for handling contact with slip and separation.
- Current mixture theories approximate perfectly bonded materials.
- Bonding often masked by low strength or material failure at the interfaces, e.g., ballistic penetration.
- Desirable attributes for the contact formulation:
  - Can be implemented in existing codes without major changes.
  - Local algorithm.
    1) No requirement for global topological information.
    2) Ease of parallelization.
  - Allows for evolving topology -- a major attraction of the Eulerian formulation.

Overview of Eulerian FEM

Lagrangian Governing Equations

- Mass:

$$\rho = \rho_0 \det\left(\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}\right)$$

- Momentum:

$$\rho \dot{\boldsymbol{u}} = \nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{b}$$

- Energy:

$$\dot{e} = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}} - \nabla \cdot (\kappa \nabla T)$$

Lagrangian Finite Element Methods

- The standard in solid mechanics for industry.
- Implementation of the Galerkin method on a computer.
  - Based on the weak form of the conservation equations.
  - The computational mesh deforms with the material.
  - Extensive literature ranging from mathematics to applications.
- Advantages:
  - Accurate
  - Efficient
- Disadvantages:
  - Limited to problems with moderate deformation.
  - Topology is fixed.

Eulerian Finite Element Methods

- Evolved from Finite Difference hydrocodes.
- Advantages:
  - Handles arbitrarily large deformations.
  - New free surfaces evolve in a natural manner.
  - Phase changes and chemical reactions are readily incorporated.
  - These strengths make the Eulerian formulation attractive for micromechanics and other engineering applications.
- Disadvantages:
  - Computational cost (impact reduced by commodity computing).
  - Diffusion of solution (but far superior to rezoning methods based on interpolation).
  - Material interfaces are perfectly bonded.

No longer major issues.

Eulerian Governing Equations

- Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

- Momentum:

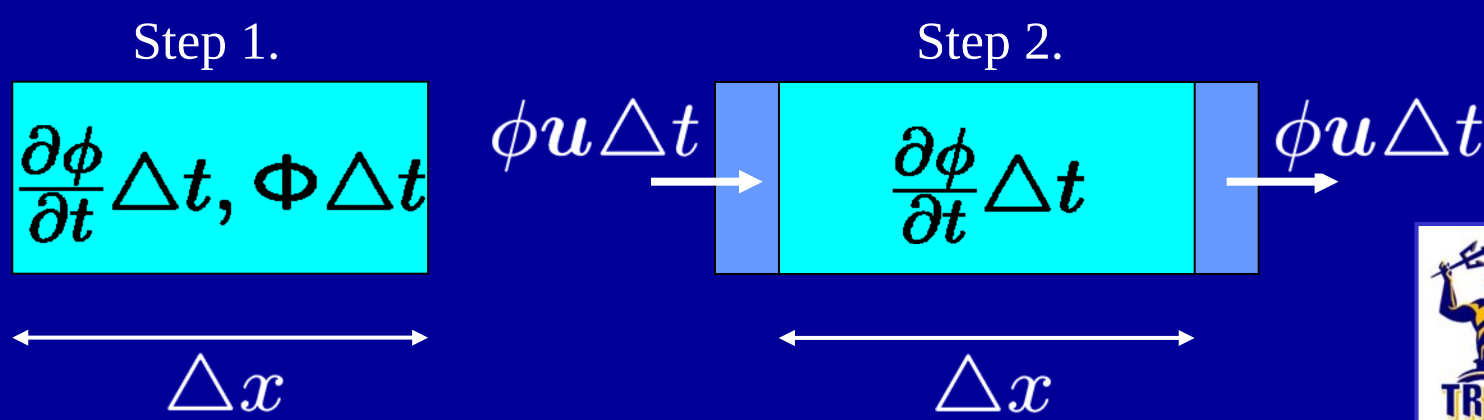
$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) = \nabla \cdot \boldsymbol{\sigma} + \boldsymbol{b}$$

- Energy:

$$\frac{\partial e}{\partial t} + \nabla \cdot (e \boldsymbol{u}) = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}} - \nabla \cdot (\kappa \nabla T)$$

Operator Splitting

	Conservation Equation	$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi u) = \Phi$
1.	Lagrangian Step	$\frac{\partial \phi}{\partial t} = \Phi$
2.	Eulerian Step	$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi u) = 0$



Explicit Lagrangian Step

Central difference integration in time
(standard practice for explicit FEM).

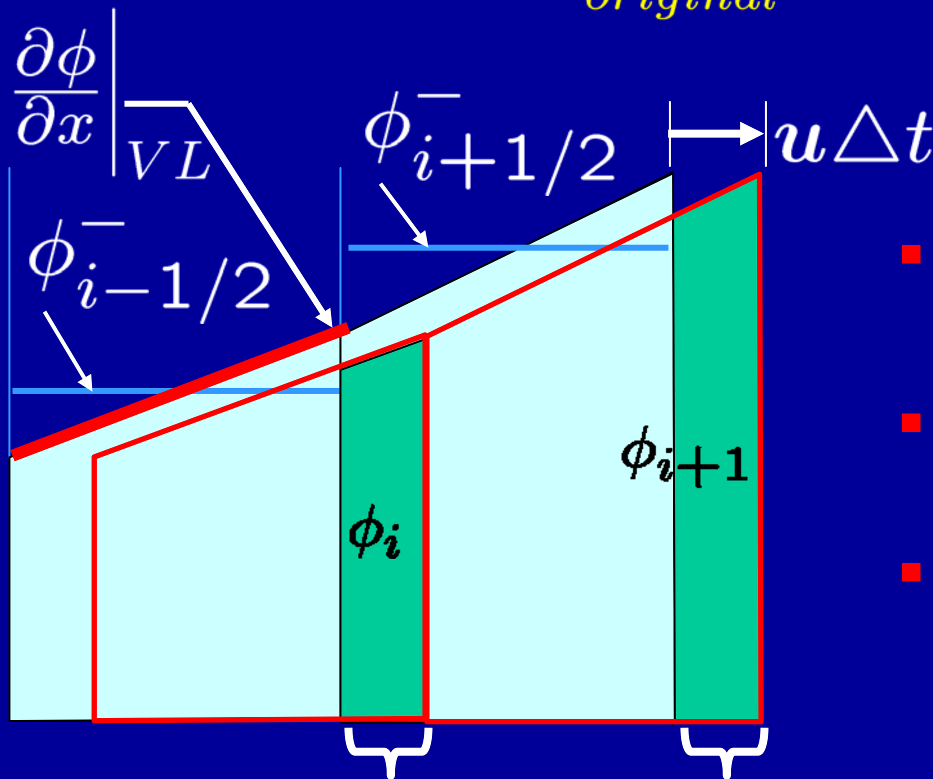
$$
\begin{aligned}
\boldsymbol{a}^n &= \boldsymbol{M}^{-1}\left\{\boldsymbol{F}^n_{external} - \int \boldsymbol{B}^T\boldsymbol{\sigma}^n dV\right\} \\
\boldsymbol{u}^{n+1/2} &= \boldsymbol{u}^{n-1/2} + \triangle t\boldsymbol{a} \\
\boldsymbol{x}^{n+1} &= \boldsymbol{x}^n + \triangle t\boldsymbol{u}^{n+1/2}
\end{aligned}
$$

Remarks:

- $\boldsymbol{M}$ is diagonal –> no linear equations to solve.
- Δt is limited by stability.
- Implicit integration also implemented.

1-D Explicit Eulerian Step

$$\phi^+_{i+1/2} = (\underbrace{\phi^-_{i+1/2}V^-_{i+1/2}}_{original} + \underbrace{\phi_i V_i}_{in} - \underbrace{\phi_{i+1}V_{i+1}}_{out})/V^+_{i+1/2}$$



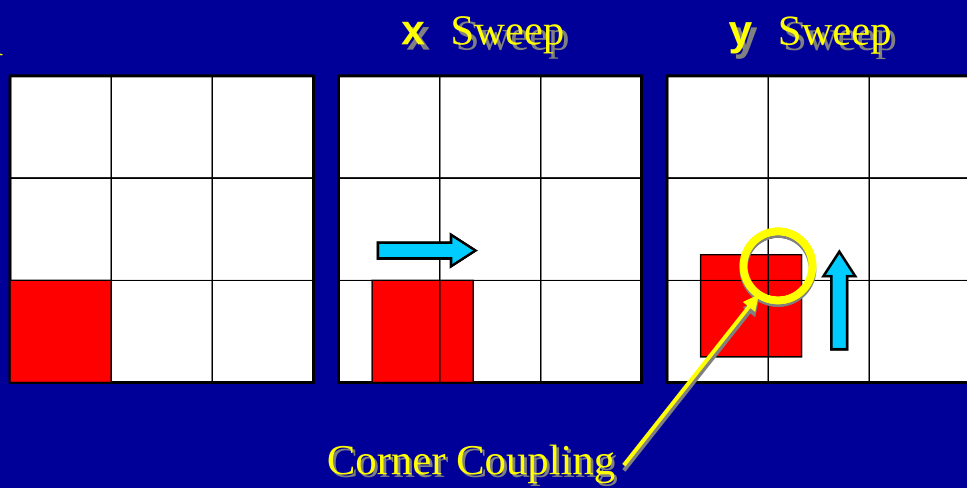
Volume transported into element i

Volume transported out of element i

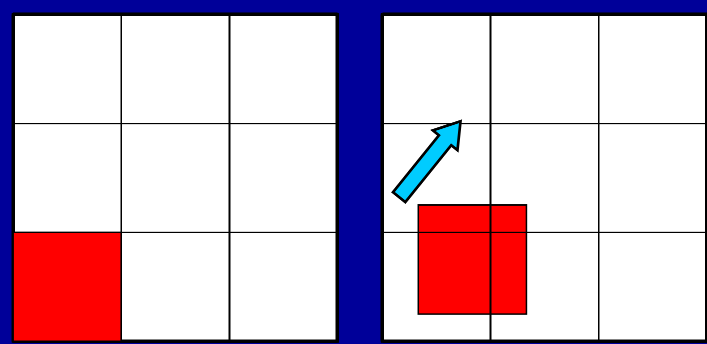
- Lagrangian Step: produces mean values of solution variables.
- Donor Cell Transport: uses mean values but only 1st order accurate.
- Van Leer MUSCL: calculates monotonic slopes from mean data. 2nd order accurate in smooth regions & 1st order monotonic at discontinuities.

Two-Dimensional Eulerian Step

- Most transport algorithms based on alternating direction methods (operator splitting).
  - Simple method for corner coupling.
  - Difficult to implement on unstructured meshes (alternating spatial directions).



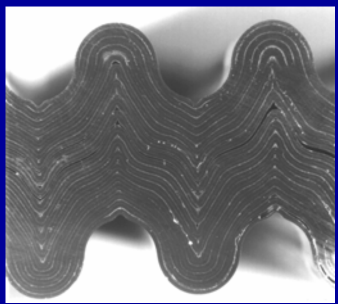
- Unsplit methods are gaining in popularity.
  - More complicated.
  - Greater cost.
  - Better accuracy with careful implementation.



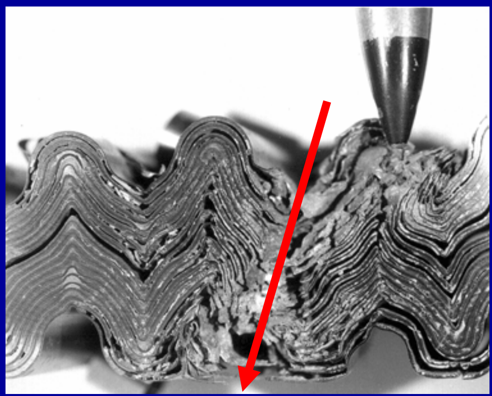
Example Eulerian Applications Where Contact is Important

Direct Numerical Simulation of a Metallic-Intermetallic Composite

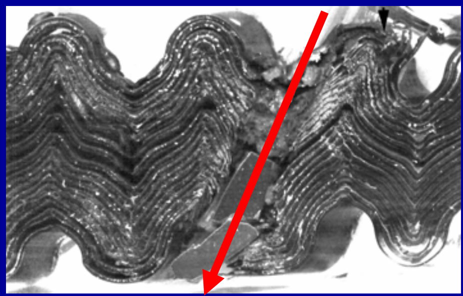
- Material prepared and tested by Ken Vecchio.
- Both projectiles are deflected by the material from their original trajectories.
- Fundamental issue: What causes the deflection?
  - Laminate structure
  - Angle of impact



MIL Before Test



.308 Penetrator

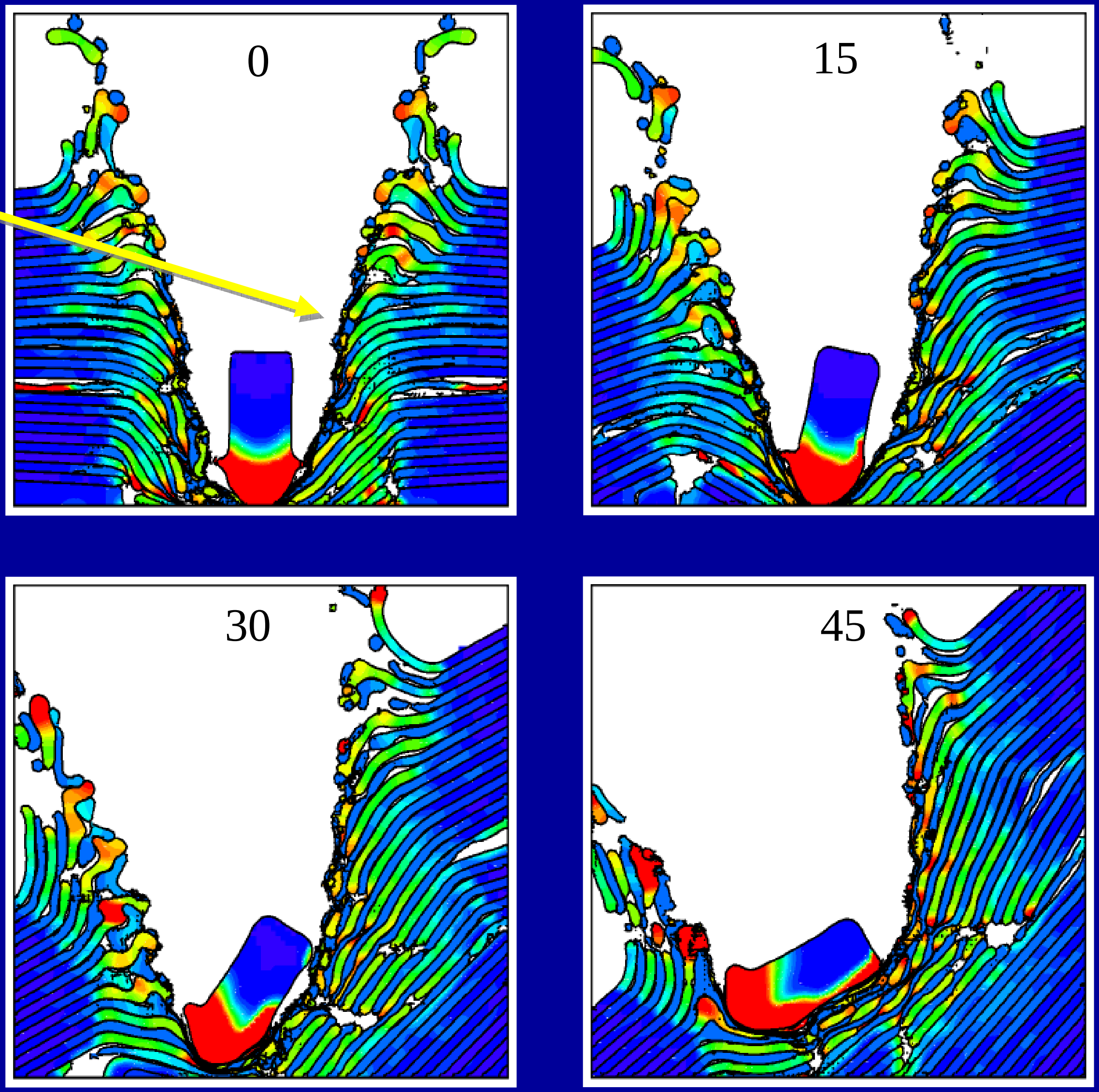


WHA Penetrator

Effect of Angle on Response

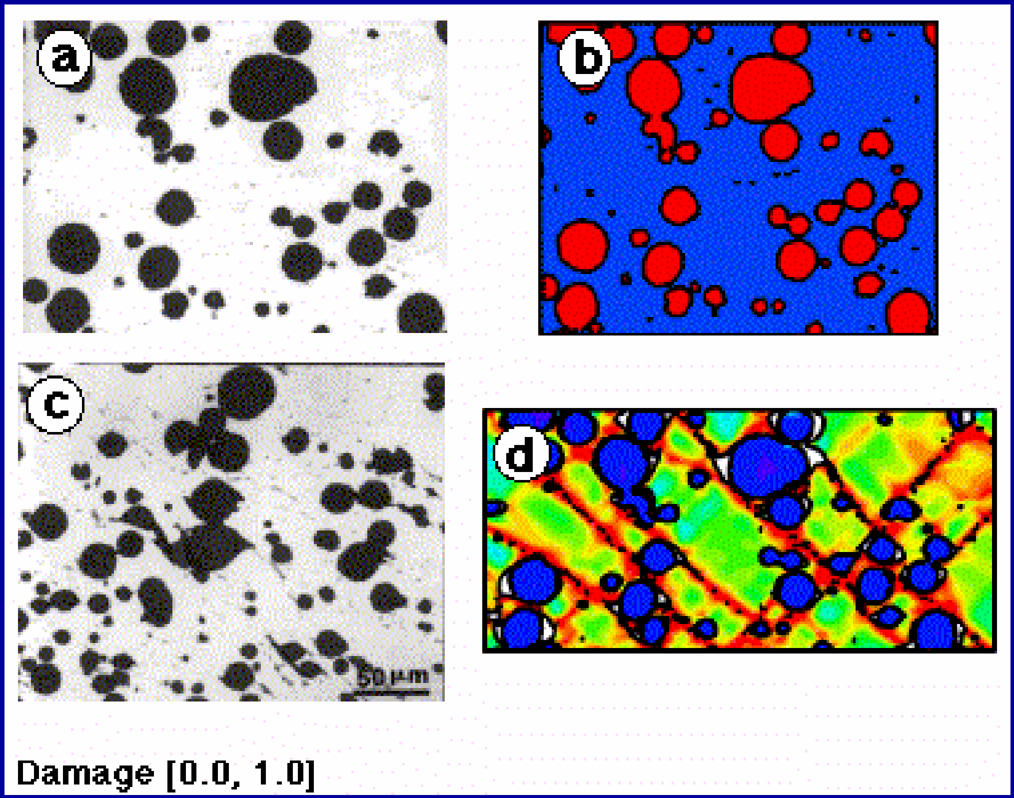
Spurious surface shear due to mixture theory.

Would be worse except for the failed material at the contact interface.

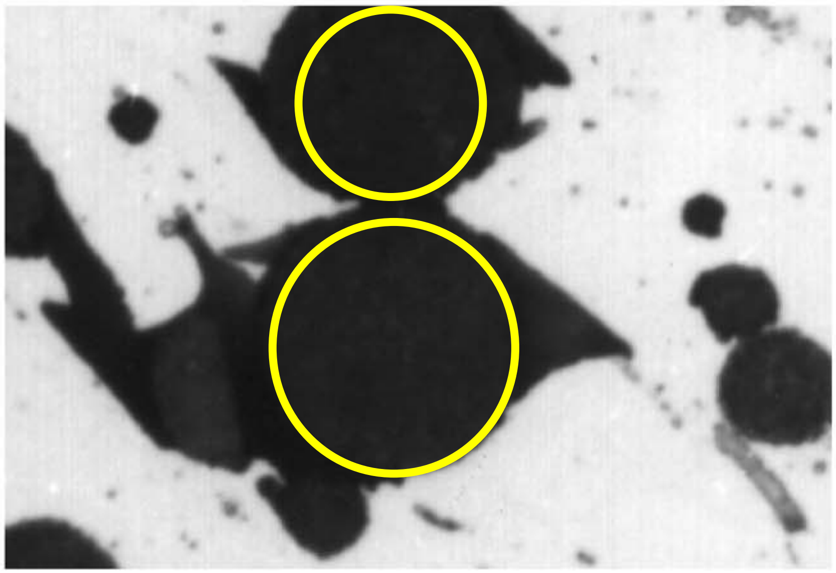


Experimentally Acquired Microstructures

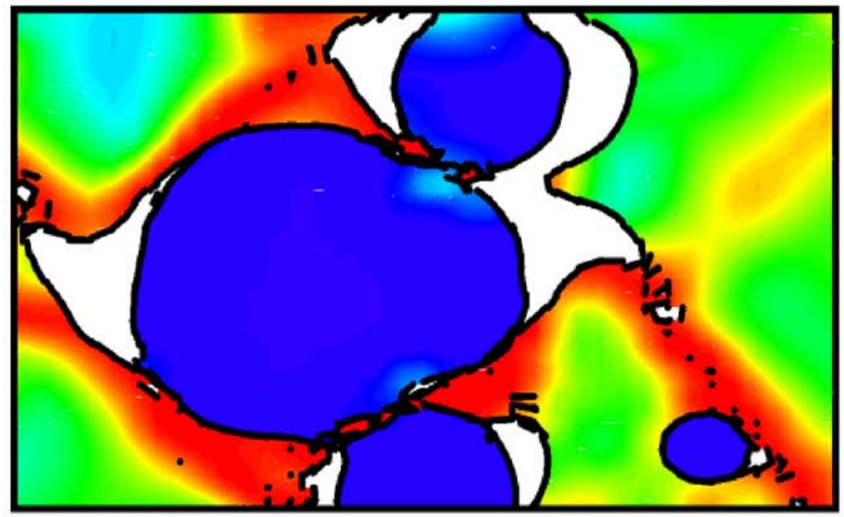
- Generating realistic synthetic microstructures is frequently challenging.
- The logically regular mesh of an Eulerian hydrocode simplifies importing digitized images.
- Example: Metal matrix composite of aluminum and alumina inclusions subjected to a compression test. Experiments performed by Prof. K. Vecchio, UCSD.



Experimentally Acquired Microstructures



Experiment

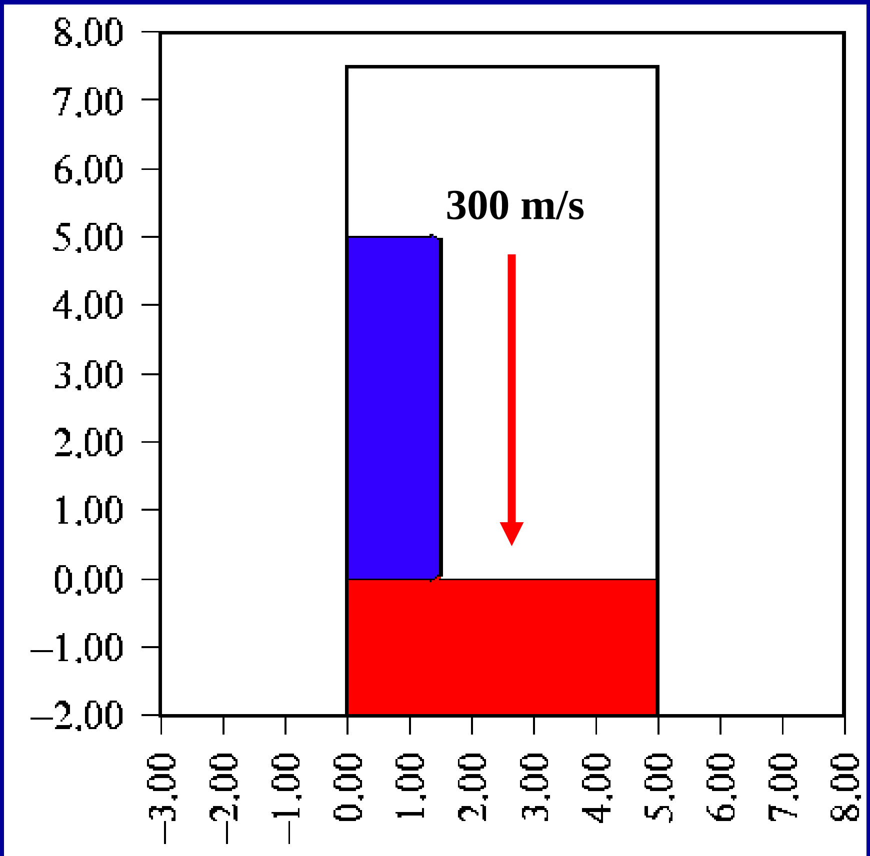


Mesoscale Simulation

Analysis was performed using the contact mixture theory. Results with simpler theories were unsatisfactory. While there is contact and separation, the relative slip between surfaces is relatively small.

X-FEM for Contact

Model Contact Problem: Taylor Bar Impact



- Elastic-plastic bar strikes elastic target at 300 m/s.
- Plane strain for maximum mushrooming of the projectile.
- Projectile properties:

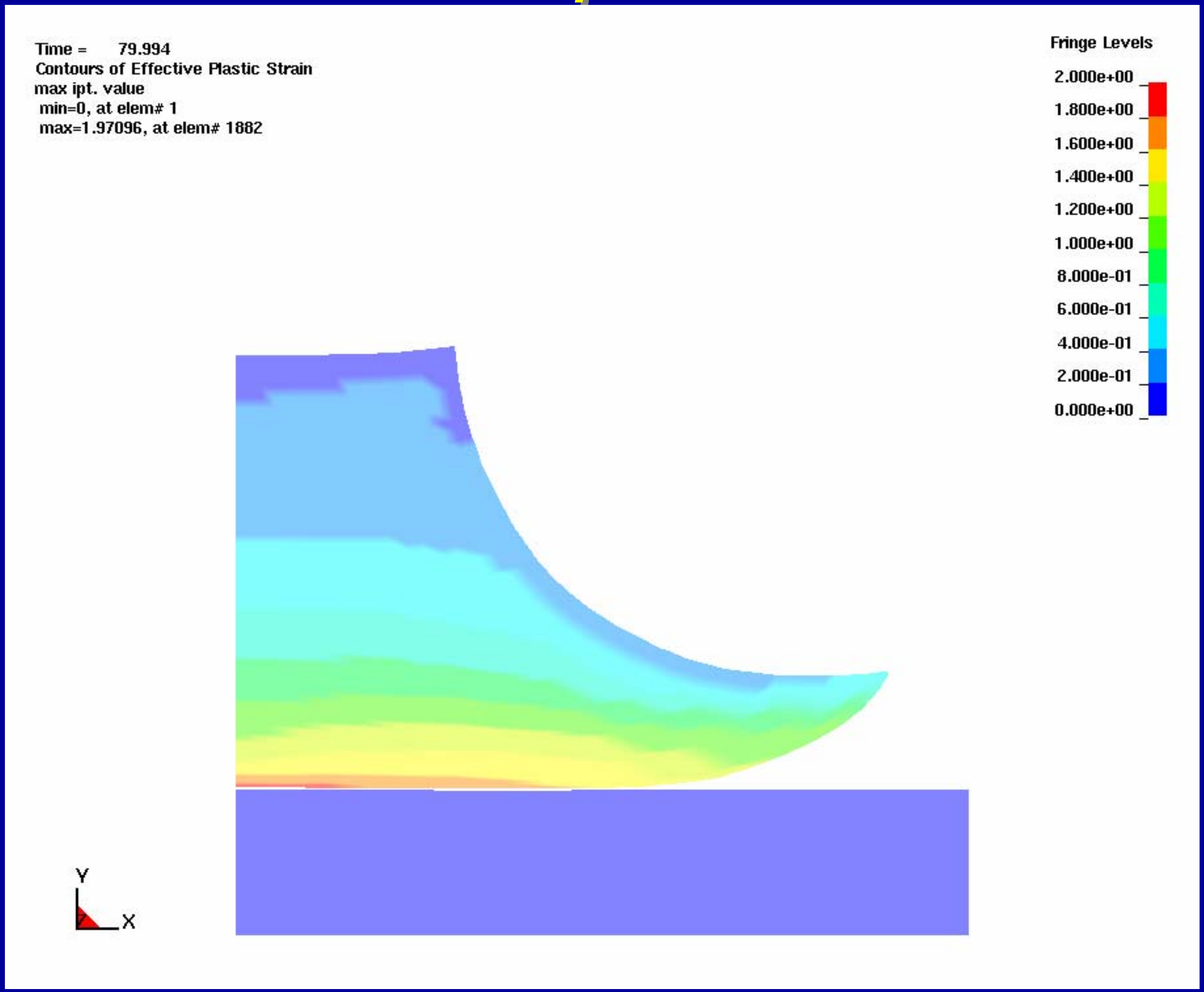
$$\rho = 1.71 \quad G = .085$$

$$\sigma_y = 2 \times 10^{-4}$$

$$h = 1 \times 10^{-3}$$

- Target is elastic with density and elastic properties 10 times higher.

LS-DYNA Lagrangian Result
Reference Solution

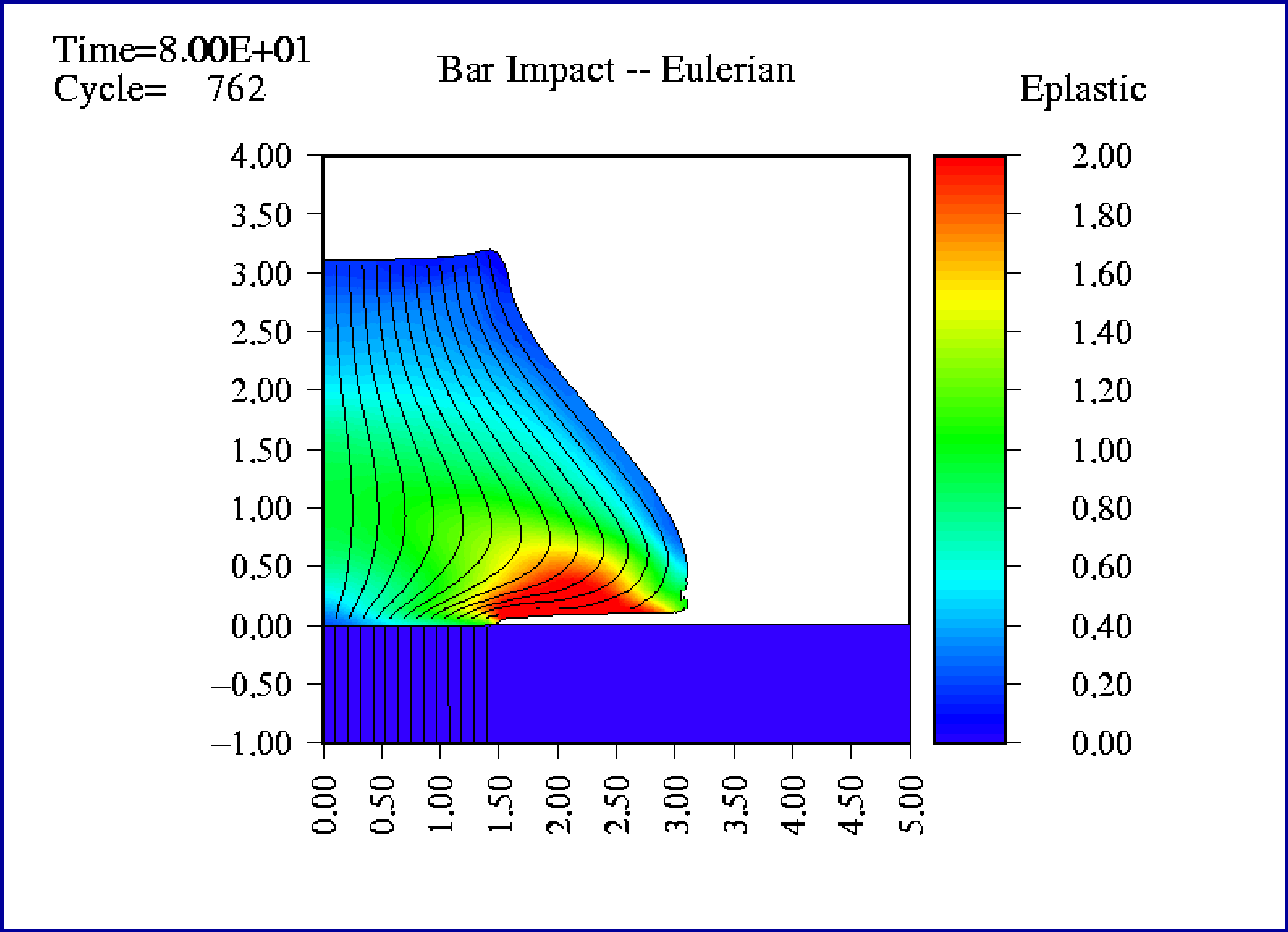


Mesh: 18 x 67 elements
Final height: 2.89
Bottom width: 4.468
Peak plastic strain: 1.97

Mixture Theories

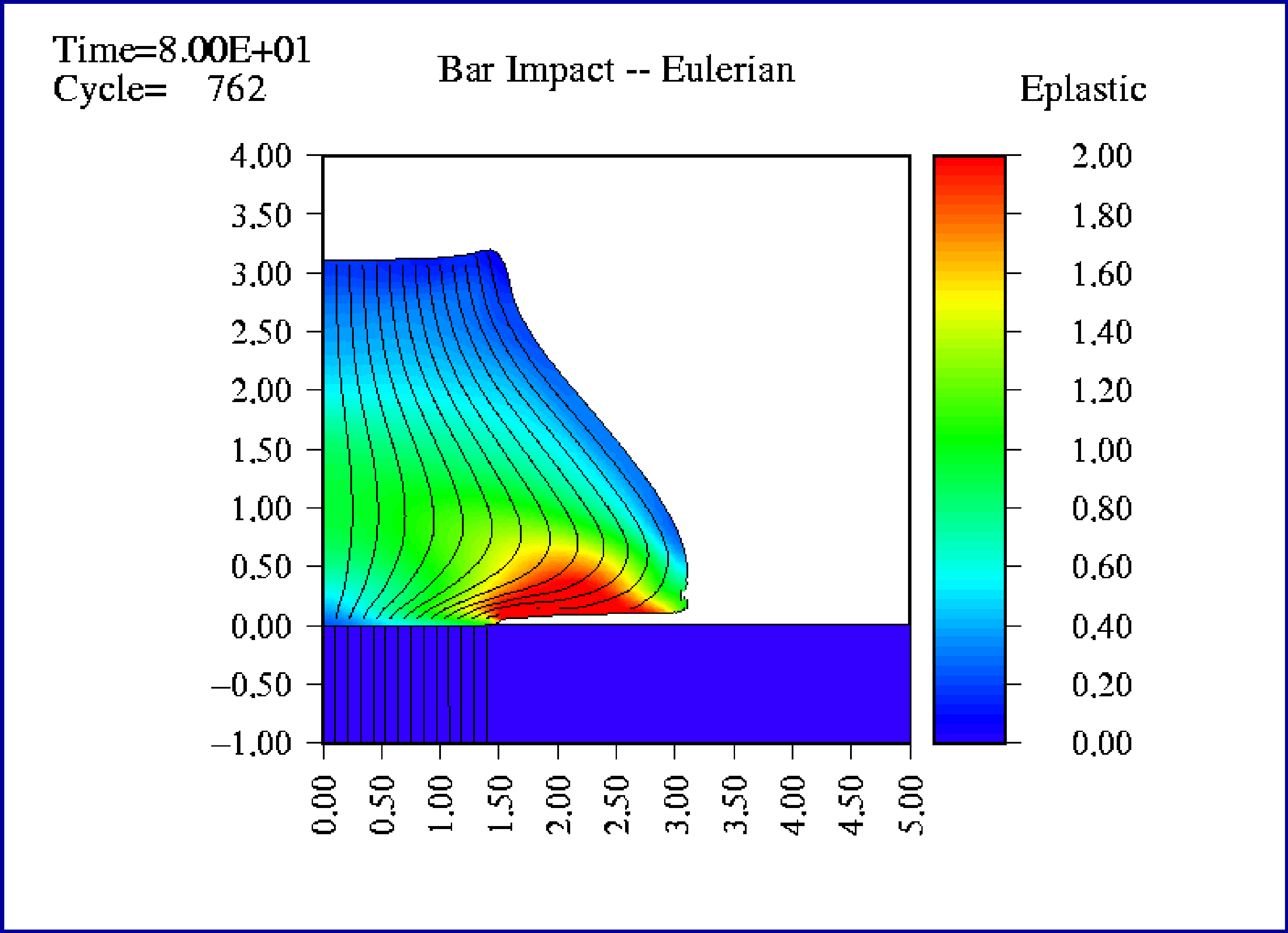
- Mixture theories are applied to elements containing more than one material (“mixed” or “multi-material” elements).
  1. Partition the strain increment between materials.
  2. Evaluate stress for each material.
  3. Calculate element stress from the material stresses.
- All interactions between materials occur in mixed elements $\longrightarrow$ the mixture theory has the role of a contact algorithm in traditional multi-material Eulerian formulations.

Mean Strain Rate Mixture Theory



Contours show original coordinates.

Zero Deviatoric Stress in Mixed Elements



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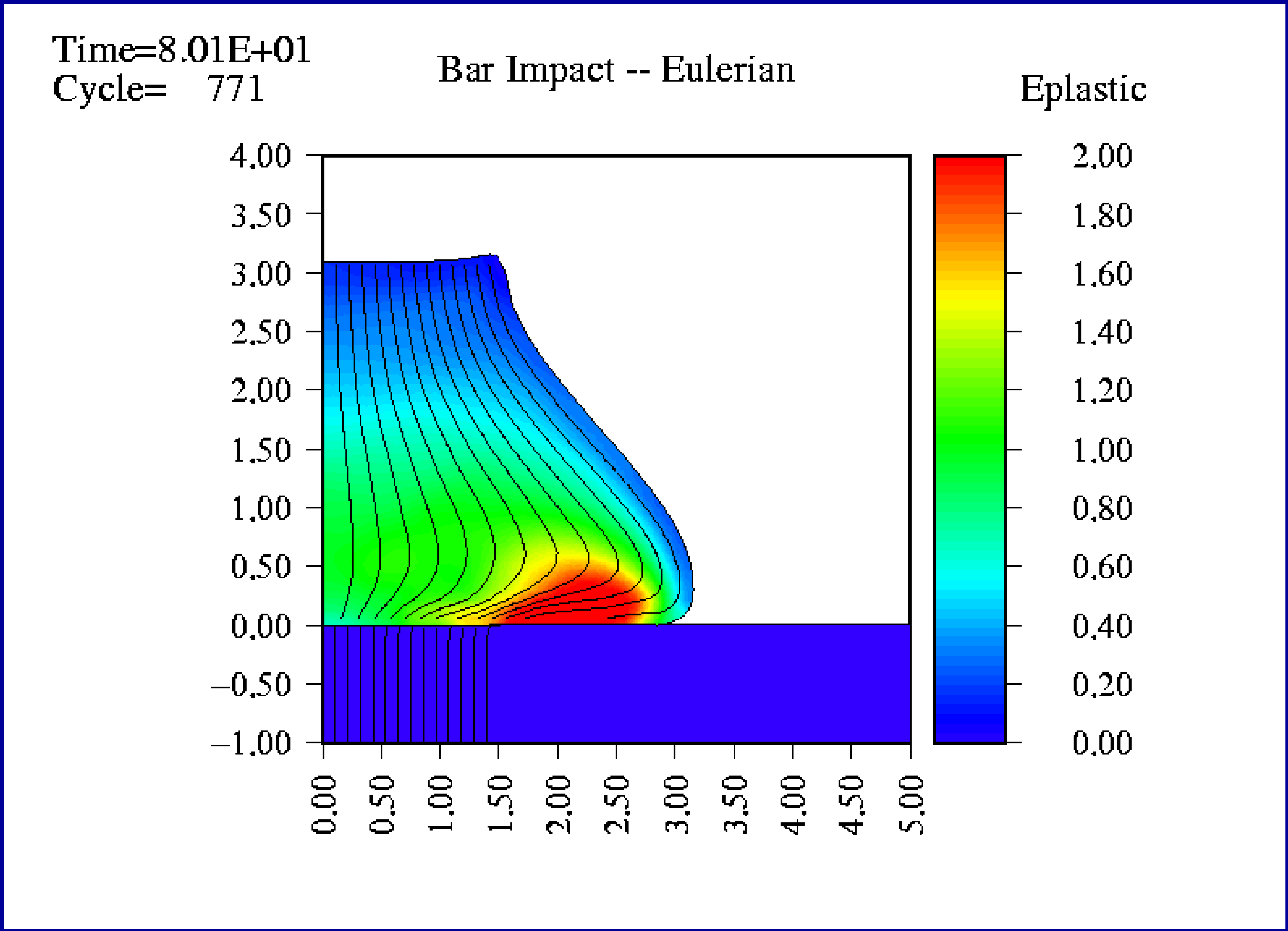
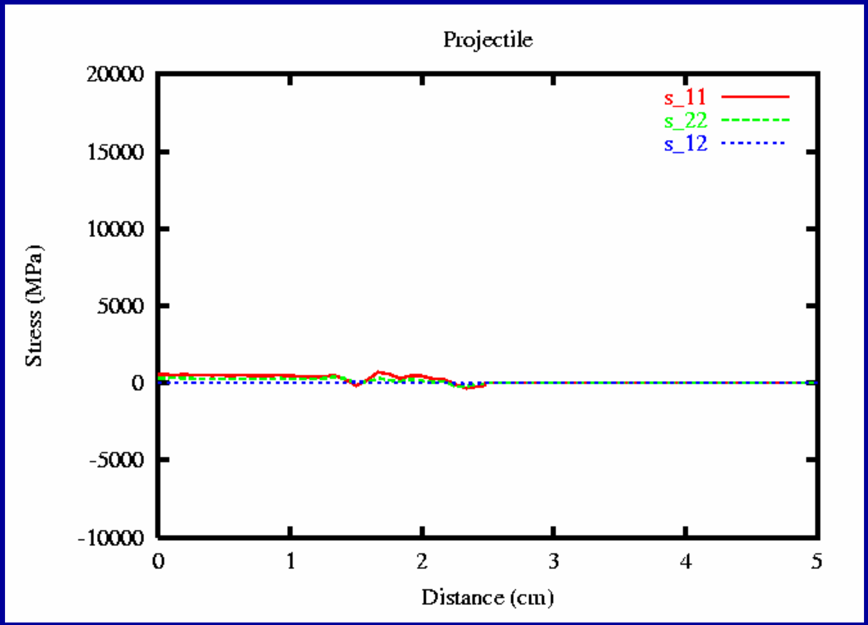
Contact Mixture Theory



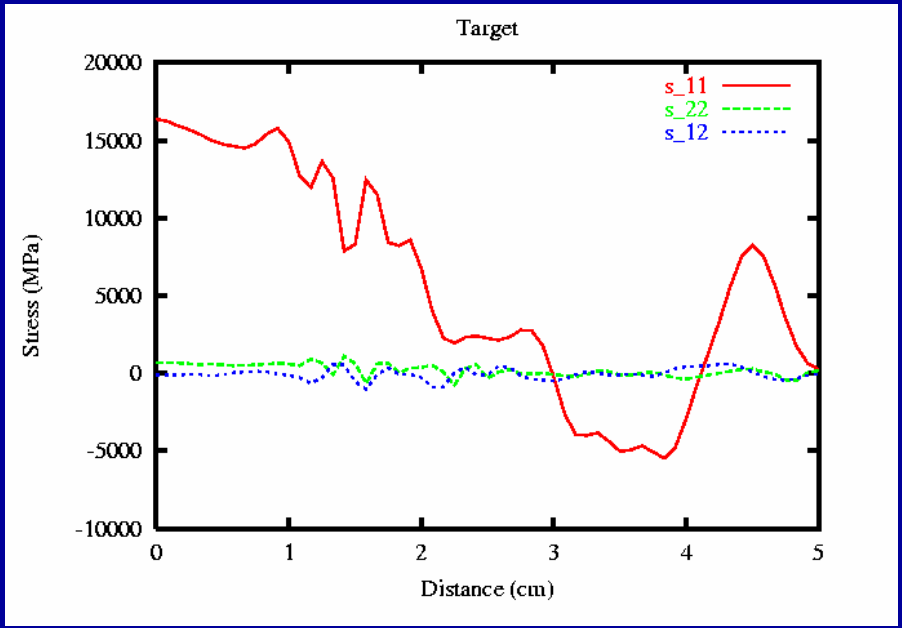
Contours show original coordinates.

What is Wrong With the Mixture Theory?

Elastic-Plastic Projectile

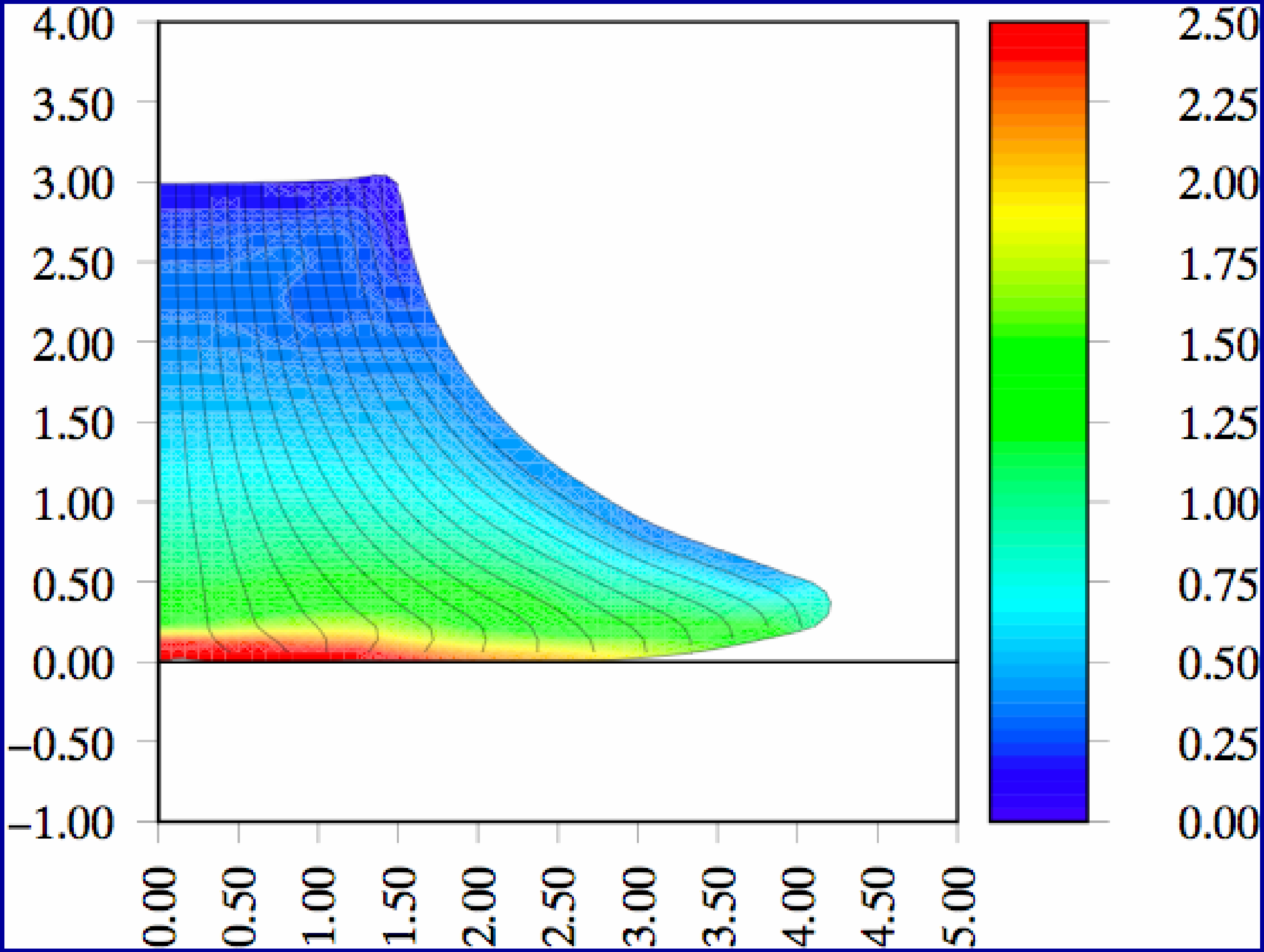


Elastic Target



- σ_{12} (free slip) and σ_{22} (limited by lowest yield stress and continuous across interface) are near zero at the interface.
- σ_{11} is
  - Limited by the yield stress in the projectile.
  - Large in the elastic target.
  - Strain rate D_{11} is the same for both the target and projectile (not governed by jump conditions).

Coupled Rigid Body - Eulerian



Contours show original coordinates.

Can be improved significantly by changing the penalty stiffness, spacing of nodes, etc.

New Eulerian Contact Approach: X-FEM

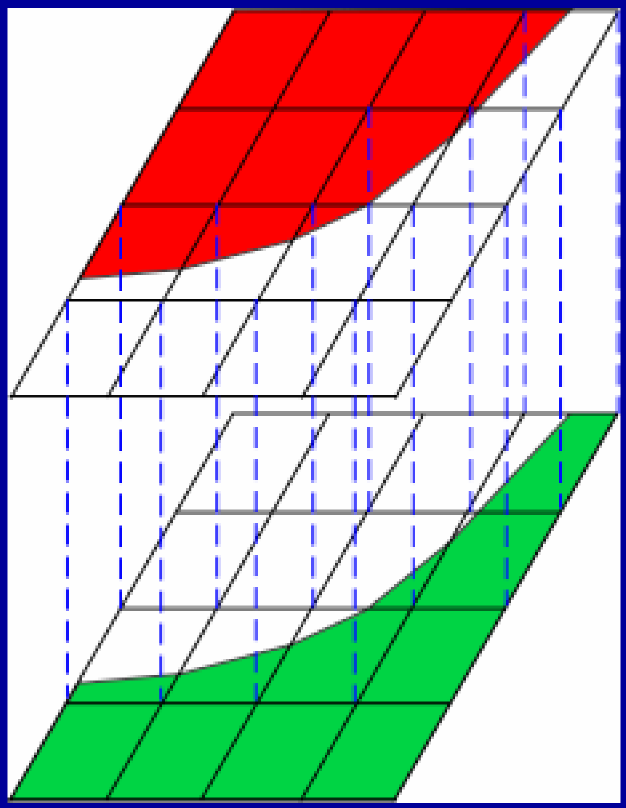
Local Enrichment of the Velocity Field

- Results shown here are preliminary.
- Developed by Belytschko et. al.
- Degrees of freedom g_j added locally to enhance accuracy.
  - Typical application is fracture. Enrichment functions approximate near tip strain field and free surface of crack.
  - Generates compatible displacements.

$$u = \sum_A N_A(x) \left(u_A + \sum_j \Psi_j(x) g_j \right)$$

X-FEM: Local Enrichment of the Velocity Field

- Nodes surrounding all the mixed elements are enriched to include for each material independent:
  - Accelerations & Forces.
  - Velocities.
  - Coordinates.
  - Masses.
- Mixed nodes are handled with data structures and algorithms similar to those for mixed elements.



X-FEM: Local Enrichment of the Eulerian Velocity Field

- At the beginning of time step *n*, the Lagrangian coordinates for each material coincide with the Eulerian mesh coordinates.

$$x^m = x^E$$

- With an element, the velocity and displacement of each material *m* is interpolated independently.

$$u^m = \sum_A N_A(x) u_A^m$$

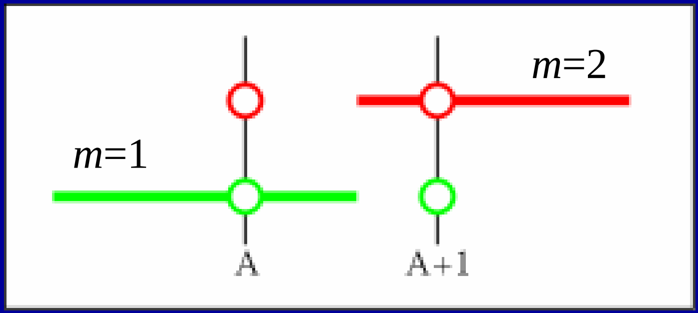
- The strain rate for each material is calculated using its own velocity field.

$$\dot{\varepsilon}^m = B v^m$$

- The stress for each material is updated using the material's strain rate.
- Unlike other X-FEM applications, need to enforce contact constraints for compatible displacements.

Enforcing the Contact Inequality

- Objectives:
  - Response normal to the contact surface is unchanged from standard Eulerian formulation.
  - Decouple response in tangential direction.
- Motivate contact enforcement in the normal direction based on a one-dimensional model problem.



$$\dot{v}_A = \frac{F_A^1 + F_A^2}{M_A^1 + M_A^2} \longrightarrow \begin{array}{l} \tilde{F}_A^m = M_A^m \dot{v}_A \\ \tilde{F}_A^m = \dfrac{M_A^m}{M_A^1 + M_A^2}\left(F_A^1 + F_A^2\right) \end{array}$$

Enforcing the Contact Inequality

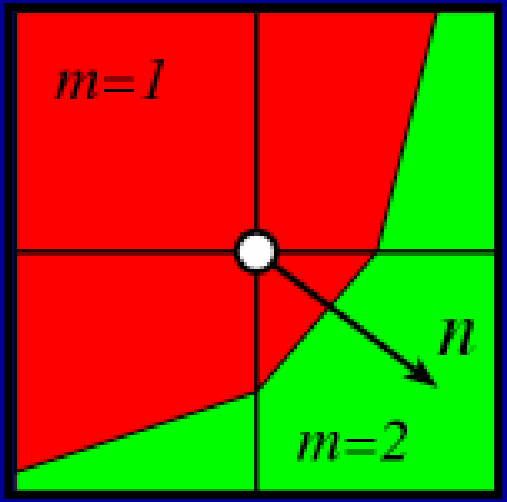
Multiple Dimensions

$$F^{TOT} = \sum_m F^m \qquad M^{TOT} = \sum_m M^m$$

$$P = n \otimes n$$

$$F^n = P \cdot F^{TOT} \qquad F^{\perp} = [I - P] \cdot F^m$$

$$\tilde{F}^m = \frac{M^m}{M^{TOT}} F^n + F^{\perp}$$

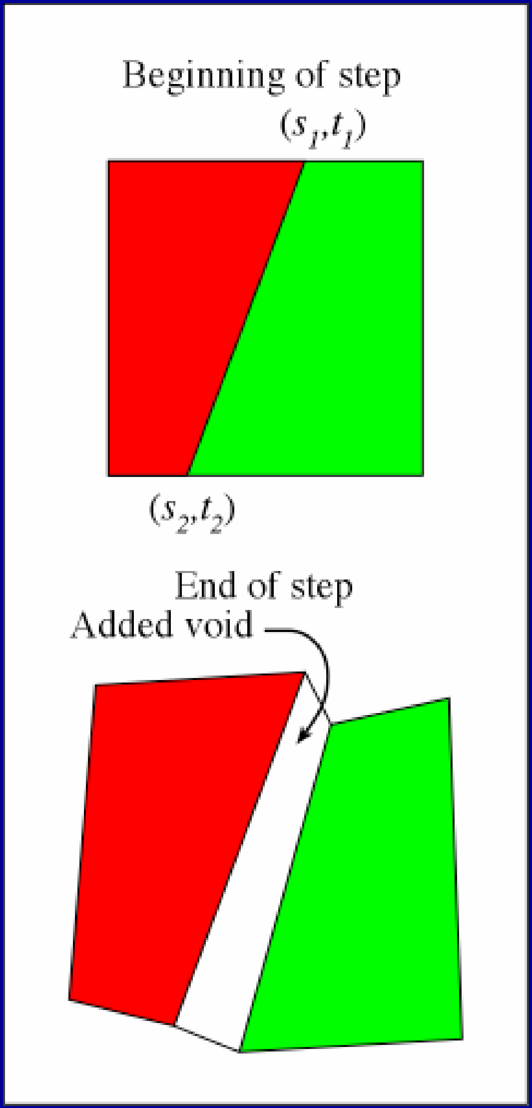


Separation Condition

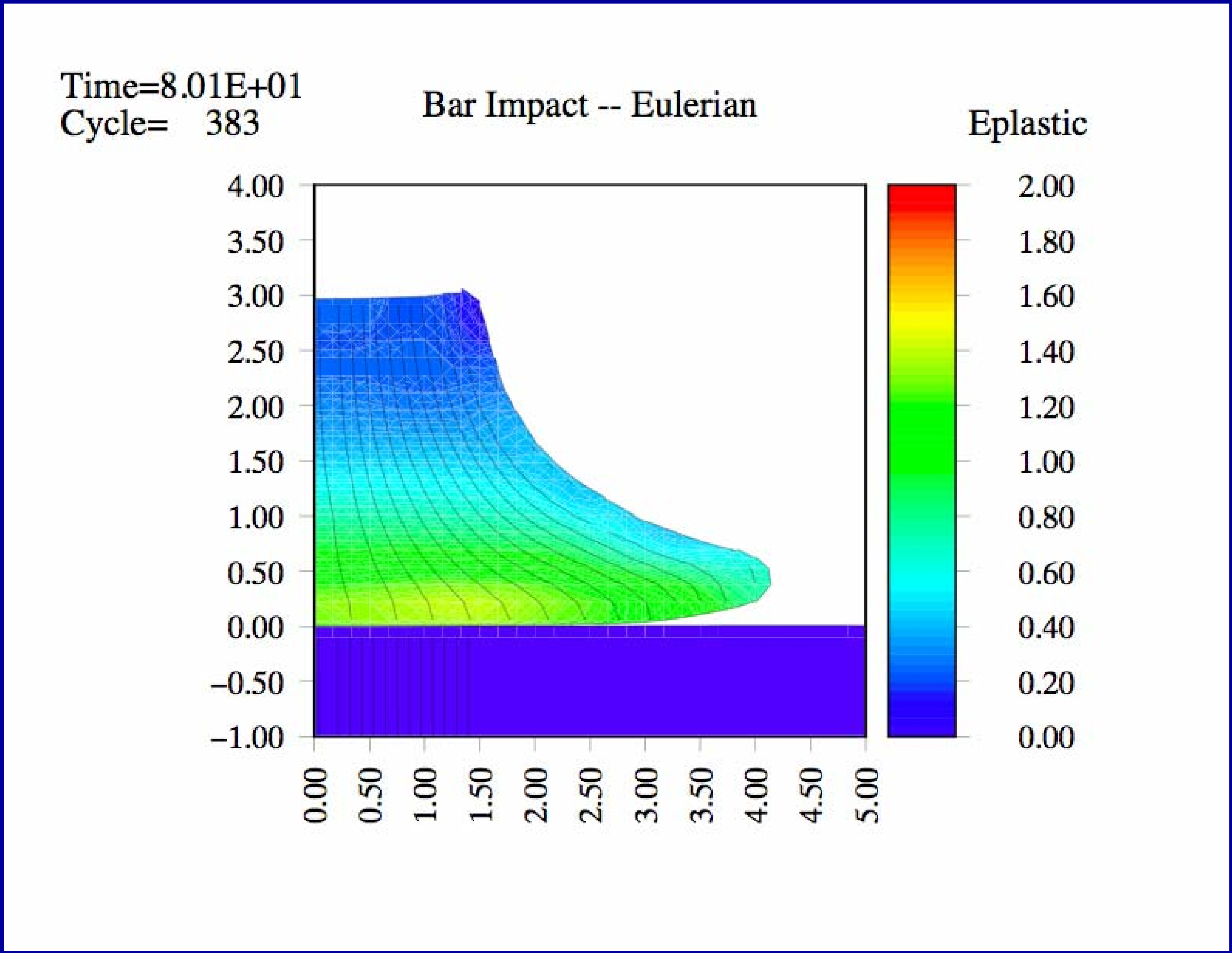
$$\text{IF } n \cdot \bar{\sigma} \cdot n \geq 0 \longrightarrow \tilde{F}^m = F^m \qquad \bar{\sigma} = \sum_{i=1}^{4} \sum_m \sigma_i^m V_i^m$$

Separation: Preparing for the Eulerian Step

- When surfaces separate, void must be introduced.
- The intersections of the interface with the element boundaries are calculated in terms of the isoparameteric coordinates (*s*,*t*) at the beginning of the time step.
- The volume generated by the surfaces at the end of the time step is calculated, and the appropriate amount of void material is added to the element.



X-FEM Coarse Mesh Result

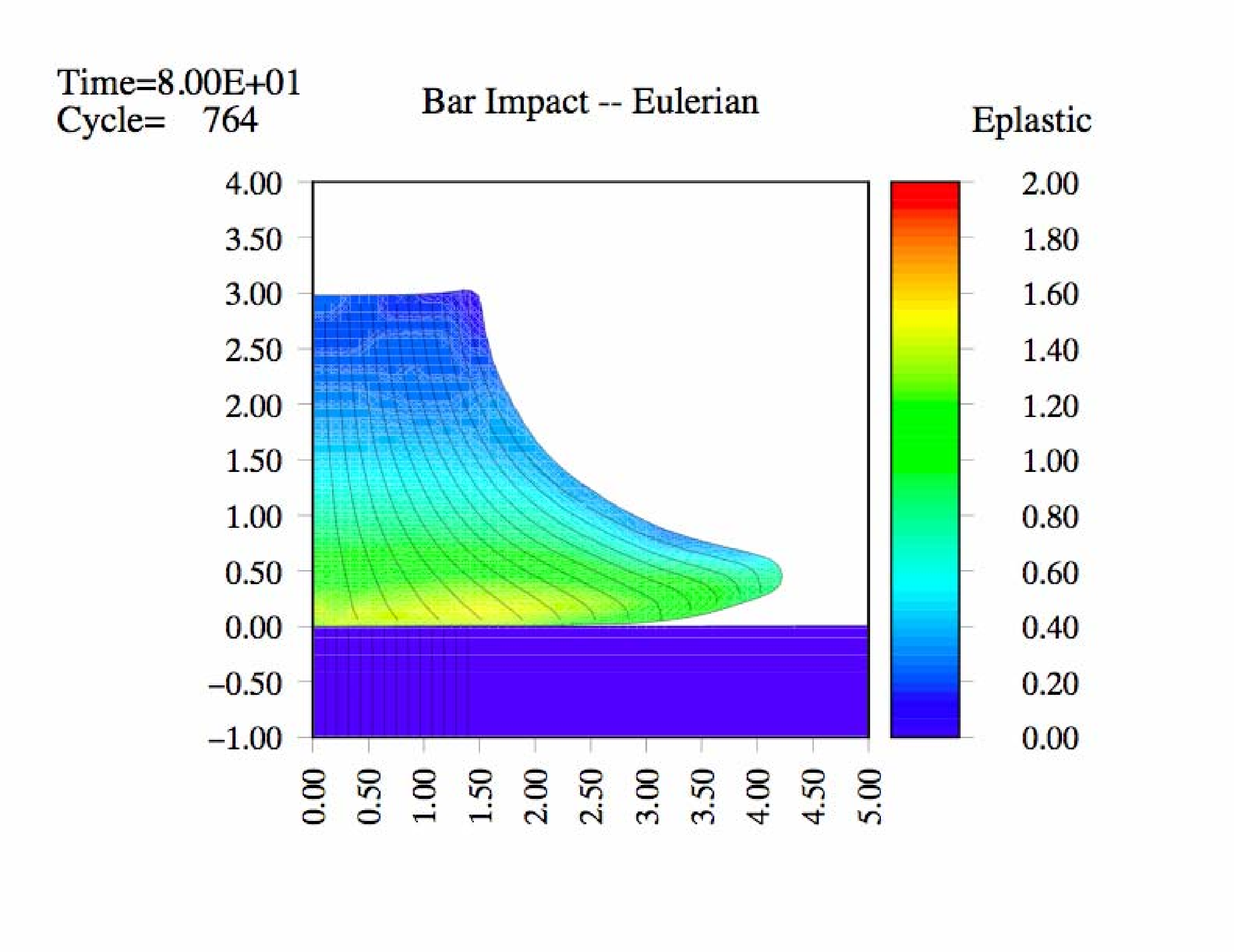


Contours show original coordinates.

Initial bar mesh resolution: 9x25

Peak plastic strain: 1.4

X-FEM Fine Mesh Result



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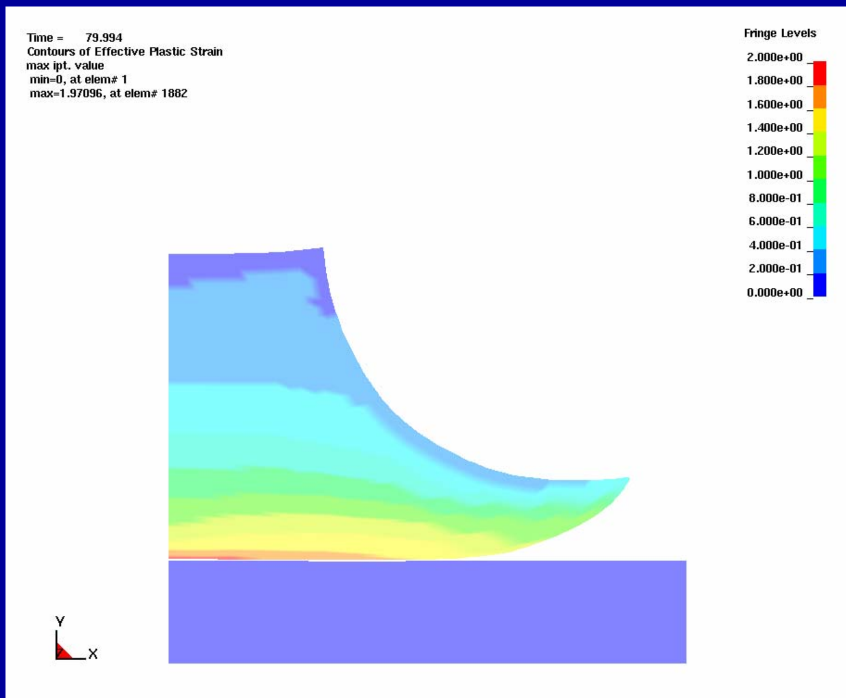
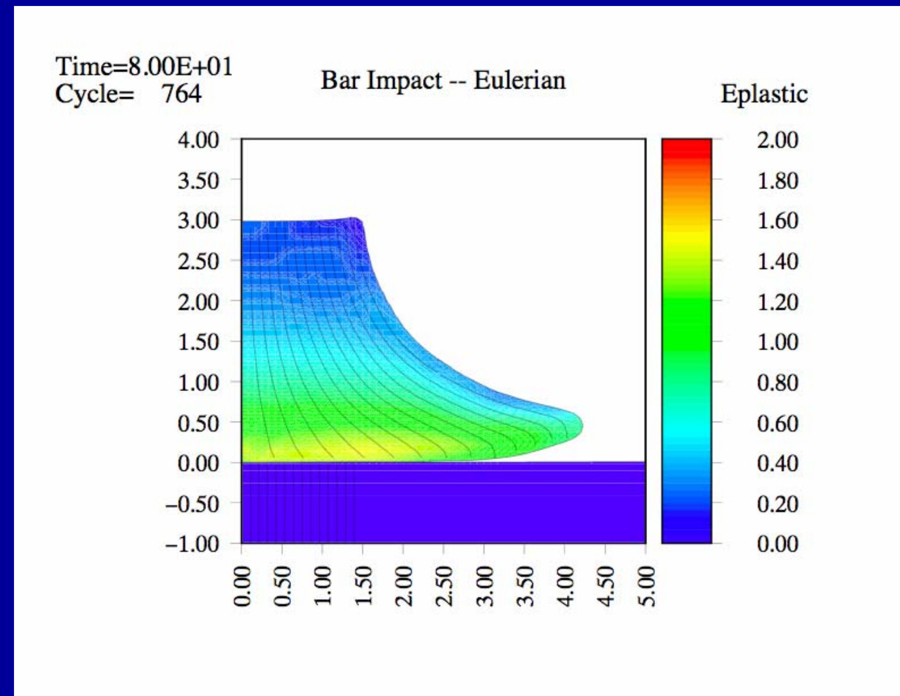
Initial bar mesh resolution: 18x50

Peak plastic strain: 1.6

Comparison of Lagrangian and Eulerian Solutions

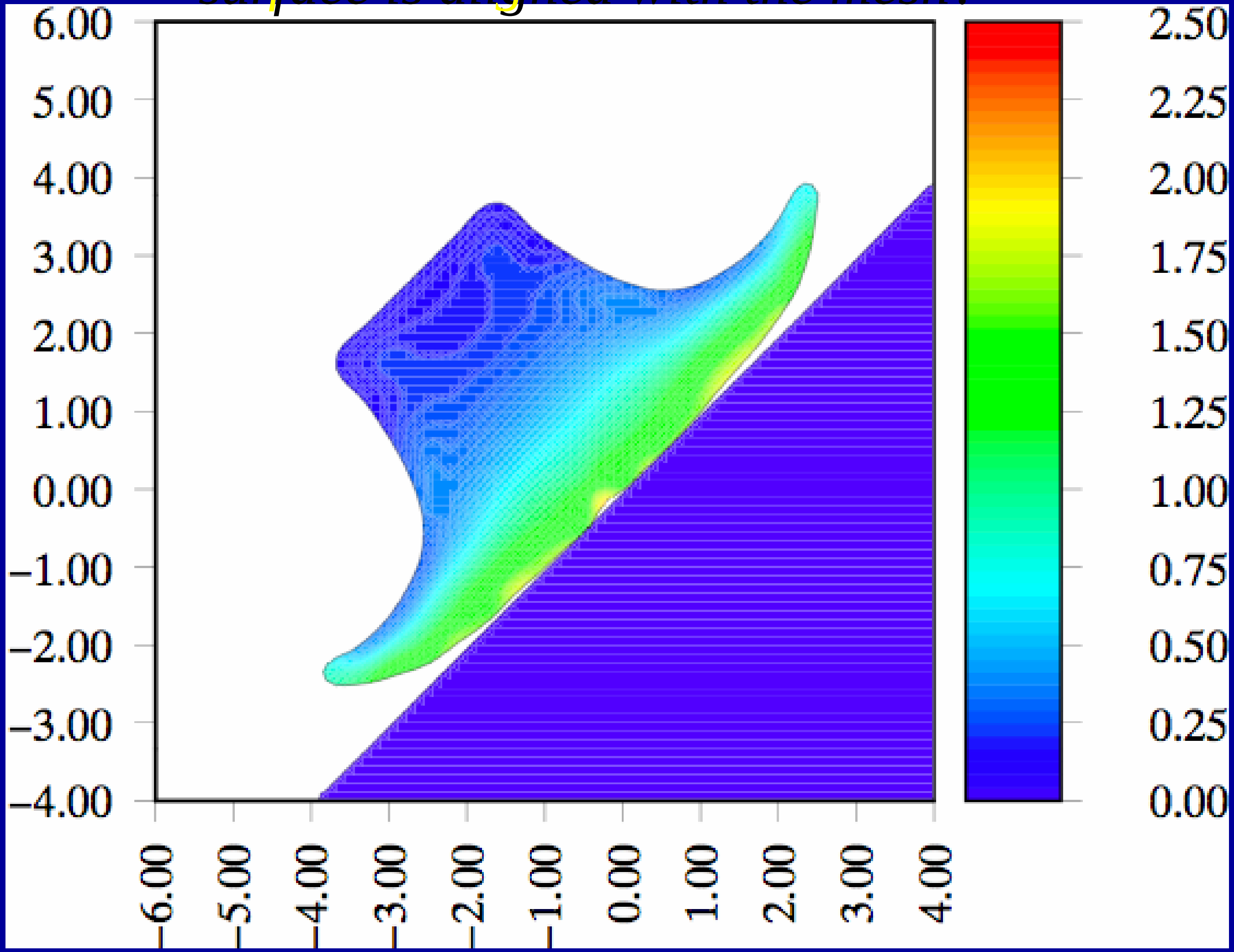




- Overall response is similar.
- Initial spatial resolution is similar: 18 x 50~70.
- Spatial resolution at late times:
  - Lagrangian is finer vertically.
  - Eulerian is finer horizontally.
- Peak plastic strains are close.

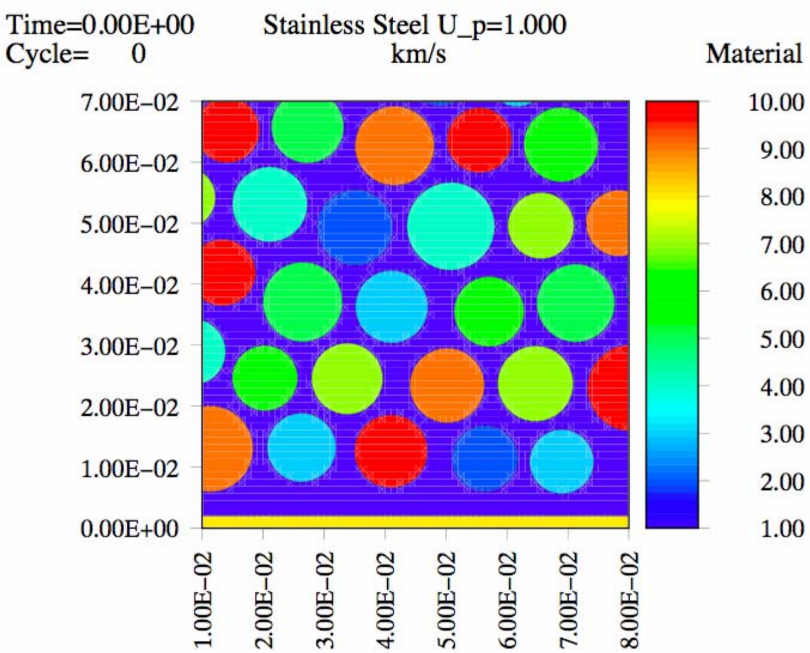
X-FEM at an Angle

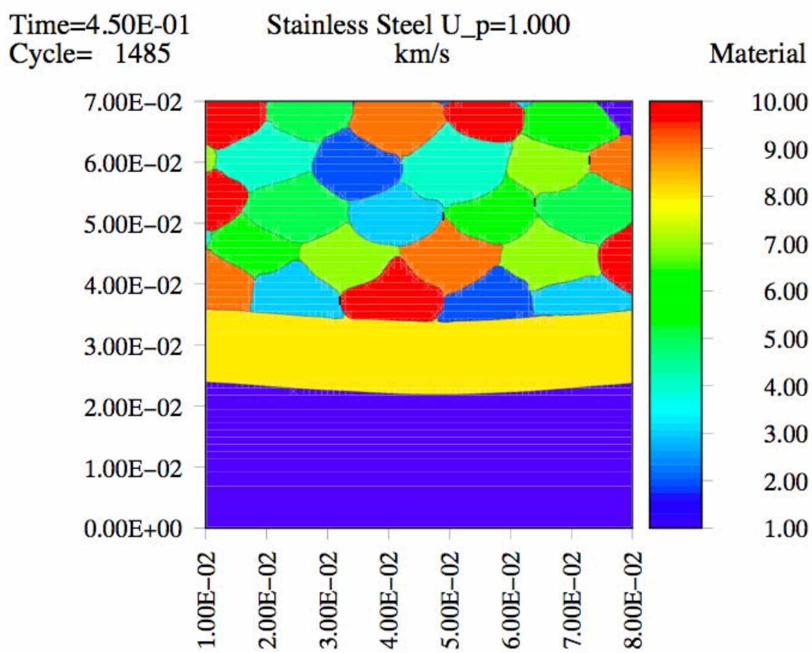
Does the X-FEM formulation only work when the contact surface is aligned with the mesh?



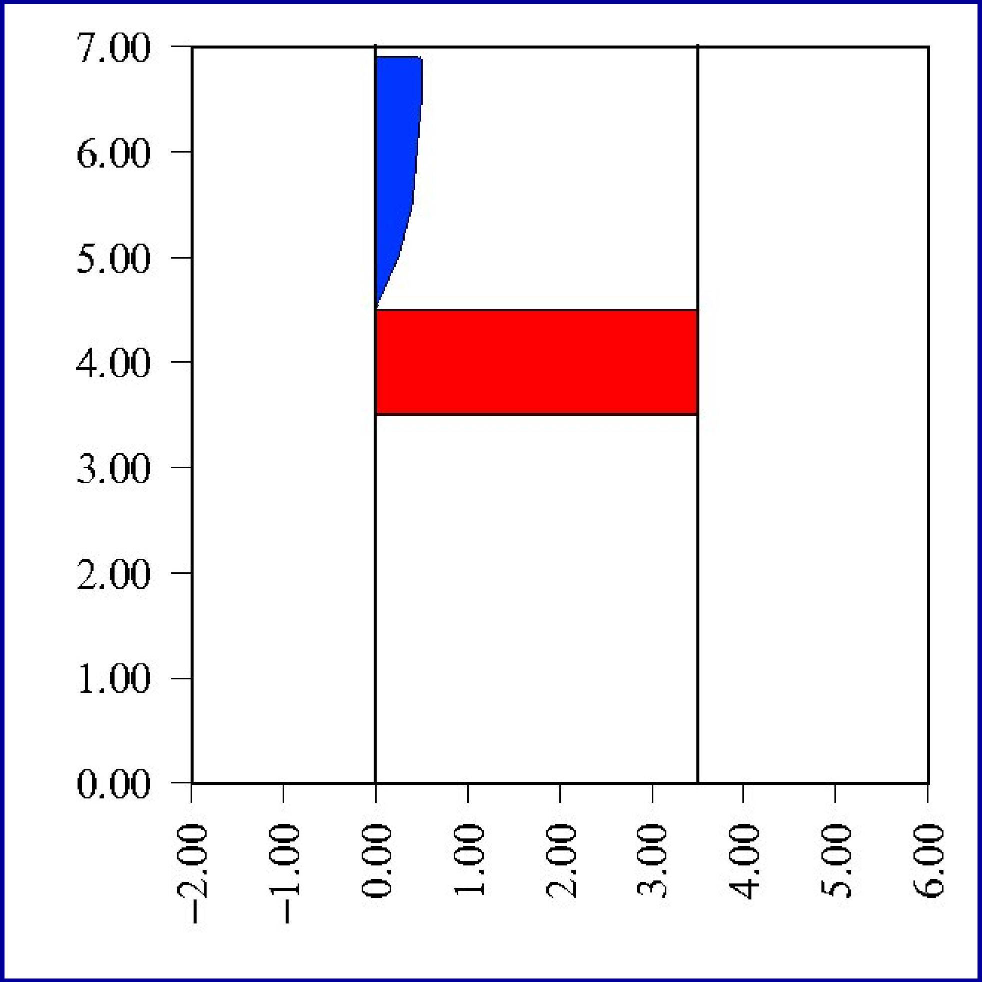
Powder Compaction

Large number of materials



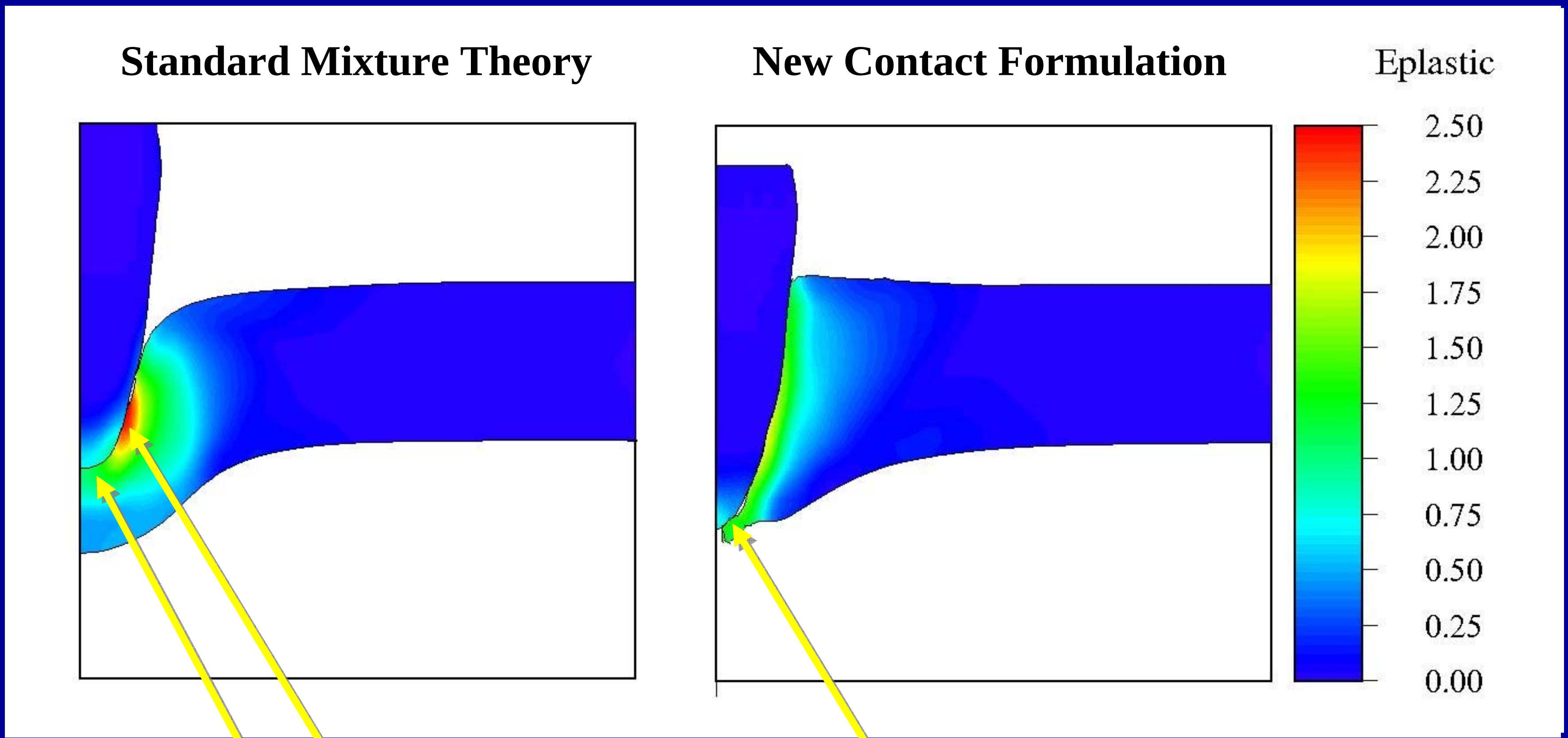


Ballistic Penetration



- Steel projectile.
  - 340 m/s initial velocity.
  - 1 cm diameter.
- Copper target.
  - 1 cm thick.
- Mesh 80 x 80.

Ballistic Penetration



Plastic strain higher.

Projectile tip blunted.

Greater penetration depth.

Conclusions

- Mixture theories are limited in their ability to model contact and slip due to the limited information in a single velocity field across all materials.
- Penalty methods can give good results but
  - Require tracer particles for enforcing the contact inequality constraint.
  - Suffer from the same limitations as Lagrangian representations of the boundary in Eulerian hydrocodes.
- Enriching the velocity field via X-FEM to give each material an independent velocity field shows great promise.
  - Can be retrofitted into legacy codes.
  - Uses only local information for easy parallelization.
  - Small memory burden.
  - Eliminates the mixture theory -- materials aren't artificially equilibrated.
  - Can be generalized to include friction and slip without separation, e.g., grain boundary slip in nanocrystalline materials.